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LABORATOIRE



INFORMATIQUE, SIGNAUX ET SYSTÈMES
DE SOPHIA ANTIPOLIS
UMR 6070

AN OPTIMIZED WORKFLOW ENACTOR FOR DATA-INTENSIVE GRID APPLICATIONS

Tristan Glatard, Johan Montagnat, Xavier Pennec

Projet RAINBOW

Rapport de recherche
ISRN I3S/RR–2005-32–FR

Octobre 2005

RÉSUMÉ :

Les applications orientées données bénéficient d'un parallélisme de donnée intrinsèque qu'il est nécessaire d'exploiter pour réduire leur temps d'exécution. Ces dernières années, des grilles de données ont été développées pour permettre le traitement et l'analyse de volumes de données imposants produits par diverses disciplines scientifiques. Ces infrastructures à grande échelle sont néanmoins soumises à une utilisation intensive et l'efficacité y est d'une extrême importance. Ce papier traite de l'optimisation des gestionnaires de workflow utilisés pour déployer des applications complexes orientées données sur les grilles. Pour ce type d'applications, nous montrons comment mieux exploiter le parallélisme de données que cela n'est fait dans la plupart des gestionnaires de workflow existant. Nous présentons la conception d'un prototype qui implémente notre solution et nous montrons qu'il fournit une accélération significative en montrant des résultats sur une application réaliste de traitement d'images médicales.

MOTS CLÉS :

Grille, workflow

ABSTRACT:

Data-intensive applications benefit from an intrinsic data parallelism that should be exploited on parallel systems to lower execution time. In the last years, data grids have been developed to handle, process, and analyze the tremendous amount of data produced in many scientific areas. Although very large, these grid infrastructures are under heavy use and efficiency is of utmost importance. This paper deals with the optimization of workflow managers used for deploying complex data-driven applications on grids. In that kind of application, we show how to better exploit data parallelism than currently done in most existing workflow managers. We present the design of a prototype implementing our solution and we show that it provides a significant speed-up w.r.t existing solutions by exemplifying results on a realistic medical imaging application.

KEY WORDS :

Grid, workflow

An optimized workflow enactor for data-intensive grid applications

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Abstract— Data-intensive applications benefit from an intrinsic data parallelism that should be exploited on parallel systems to lower execution time. In the last years, data grids have been developed to handle, process, and analyze the tremendous amount of data produced in many scientific areas. Although very large, these grid infrastructures are under heavy use and efficiency is of utmost importance. This paper deals with the optimization of workflow managers used for deploying complex data-driven applications on grids. In that kind of application, we show how to better exploit data parallelism than currently done in most existing workflow managers. We present the design of a prototype implementing our solution and we show that it provides a significant speed-up w.r.t existing solutions by exemplifying results on a realistic medical imaging application.

I. CONTEXT AND OBJECTIVES

This work aims at enacting an efficient and data-driven grid-enabled workflow. We consider complex data-intensive applications for which data grids have been developed and that benefit from a workflow management system to handle the computations involved.

We are especially targeting application workflows including *several successive steps* of significant duration and made up from *generic components*. We are moreover focusing on *data-intensive* applications which are characterized by the iteration of the same workflow on many input data sets. This kind of application can be found in the medical imaging field, where applications processing large image databases through a complete sequence of generic treatments are very common [1].

In this paper, we consider that a workflow is a set of *services* interconnected with *data dependency links*. We are referring to the service-based approach of workflow composition that is briefly described in section II. A service in this sense is a logical processing unit, implemented by a specific data processing algorithm, through which input data are

transformed into output data. Figure 1 presents the graphical notations we use in the rest of the paper.

The target infrastructure for this work is a grid of standard personal computers interconnected by a high bandwidth network and managed through a super-batch scheduler such as the EGEE grid infrastructure¹. Earlier work has shown that it is possible to operate a Web-Services based workflow processing unit on top of such an infrastructure [2] but that optimal performances for data-intensive applications cannot be obtained without taking into account the data parallelism inherent to this kind of application into the scheduling policy.

We show that current technologies only partially address these requirements and we propose new methods for optimizing the workflow execution under the above assumptions by exploiting the data parallelism. Some performance results on a real data-intensive medical imaging application are shown.

Section II presents related work about workflow management systems in the e-Science field. Sections III and IV detail why and how to exploit parallelism in a workflow in order to optimize its execution on a grid infrastructure. In section V, we present an implementation of an optimized enactor prototype taking into account the points highlighted before. Section VI then presents experiments and our prototype performance results.

II. RELATED WORK

One can basically identify two approaches for workflow composition: the job-based approach and the service-based approach. These two approaches differ by the role of the workflow manager. A complete taxonomy of workflow managers for e-Science is presented in [3].

¹<http://www.eu-egee.org>

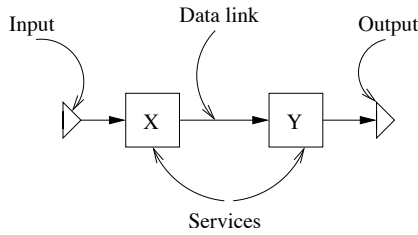


Fig. 1. Graphical workflow notations used in the paper

A. Job-based approach

In the job-based approach, the workflow manager is responsible for the actual processing of data by programs on physical resources.

The job-based approach is very close to the grid infrastructure: in this approach, the workflow manager itself submits jobs to the grid. Thus, it allows the optimization of variables such as the job submission rate, the dispatch rate and the scheduling rate as detailed in [4].

DAGMan [5] is the emblematic workflow manager of the job based approach. A Direct Acyclic Graph (DAG) describes dependencies between Condor [6] jobs. A child node is started once all its parents have successfully completed. Among other workflow managers, the Pegasus system [7] is also based on this paradigm. It takes an abstract description of a workflow (that can be constructed by using Chimera [8]) and finds the appropriate data and grid resources to execute the workflow. Other systems such as GRID superscalar [9] also identifies tasks from a sequential application including particular primitives in its code and manages their submission to a grid. The P-GRADE environment [10] also allows the creation, execution and monitoring of job-based workflows on various grid platforms.

B. Service-based approach

In the service-based approach, the workflow manager is responsible for the transmission of the data to distant services and for the collection of the results. The workflow manager is just aware of the interface of the programs and do not access the actual binary files. Jobs are submitted to the grid by the services.

In this approach, the description of a workflow is made from the interface of the programs composing the workflow. This interface describes the inputs

and outputs of a program and informs the workflow manager of how to invoke the services. Among various standards of service interface description, the Web-Services Description Language [11] is nowadays widely used in workflow management systems.

The description of the dependencies between services is expressed with a language which must be able to describe all the required patterns needed to build the workflow. A complete survey of such workflow patterns is presented in [12]. Many workflow description languages emerged from the e-Business field during the last few years and led to standardization efforts still in progress [13] [14]. In the e-Science field, initiatives tended to propose less exhaustive but simpler languages on the basis of data dependencies. Examples of such languages are the Simple Concept Unified Flow Language (Scufl) [15] and the Modeling Markup Language (MoML) [16].

Various service-based workflow management systems have been proposed in the e-Science field. Among them, the Kepler system [16][17] targets many application areas from gene promoter identification to mineral classification. It can orchestrate standard Web-Services linked with both data and control dependencies and implements various execution strategies. The Taverna project [15], from the myGrid e-Science UK project² targets bioinformatics applications and is able to enact Web-Services and other components such as Soaplab services [18] and Biomoby ones. It implements high level tools for the workflow description such as the Feta semantic discovery engine [19]. Other workflow systems such as Triana [20], from the GridLab project³, are decentralized and distribute several control units over different computing resources. This system implements two distribution policies, namely parallel and peer-to-peer. It has been applied to various scientific fields, such as gravitational waves searching [21] and galaxy visualization [20]. Recent work⁴ aims at deploying this system on the EGEE grid infrastructure.

Finally, at a higher level, describing a work-

²<http://mygrid.org.uk>

³<http://www.gridlab.org>

⁴<https://gilda.ct.infn.it/>

flow with the service-based approach may require to introduce a domain-specific ontology to facilitate automatic format conversion and services fitting [22]. Such tools are integrated into the Taverna workbench [15]. Closely to our application field, an example of a neuroimaging ontology modeling is presented in [23].

C. Comparison of the two approaches

In the service-based approach, the workflow description stipulates that a particular output of a program is to be linked to a particular input of another one. Thus, the iteration of such workflows on a number of input data sets is straightforward and does not require any rewriting of the workflow. For instance, the Taverna workbench uses so-called iteration strategies (described in section V-C) that are convenient to implement data-centric applications. On the contrary, in the job-based approach, data dependencies between programs are not explicitly described. Iterating a single workflow on many data sets thus requires to write specific jobs for each data set. Indeed, one job in the workflow exactly corresponds to one task to be submitted and computed on the grid and it cannot be instantiated with different data sets.

The service-based approach is more independent from the infrastructure than the job-based one because the services themselves are responsible for the submission of jobs to the grid whereas it is the role of the workflow manager in the job-based approach. One of the consequences is that the service-based approach allows different services included in the same workflow to submit jobs on various types of grids. It also permits the composition of applications including legacy code because the workflow manager do not even access the binary that would be executed on the grid. The service-based approach thus offers a lot of flexibility for the benefit of the user by making the sharing and reusing of generic components easier, which particularly suits to the kind of applications we are targeting.

The service-based approach is thus well-adapted to our assumptions described in section I. Nevertheless, the service-based approach makes the optimization of the computations much more complex as the workflow manager is not in direct contact with the computation infrastructure(s).

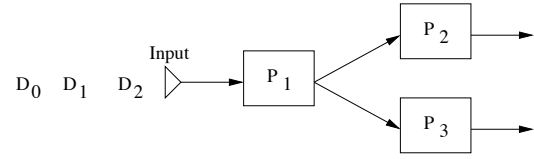


Fig. 2. A simple workflow example

The ultimate goal of this work is to optimize the execution of service-based workflows on the grid. We present here a first solution by exploiting parallelism inherent to the workflow itself, the data to process, and the services to execute.

III. PARALLELISM IN A WORKFLOW

A. Intrinsic workflow parallelism

The first trivial way of parallelism in a workflow deals with the intrinsic workflow patterns. It consists in allowing services to be enacted independently from each other when they are not linked by any kind of dependence. For example, if we consider the simple workflow pattern represented on figure 2, the service P_2 must be able to be enacted independently from the service P_3 . This kind of parallelism is implemented by the majority of workflow enactors today.

B. Data parallelism – multithreading

When considering data-intensive applications, several input data sets are to be processed according to the same workflow. Benefiting from the large number of resources available in a grid, workflow services can then be instantiated as several computing tasks running on different hardware resources and processing different input data in parallel.

Multithreading denotes that a service is able to process many data sets simultaneously with a minimal performance loss. This definition implies that multithreading can only be achieved efficiently on a multiprocessor infrastructure such as a grid. Indeed, even if the operating systems nowadays allow simultaneous processings on a single processor, increasing the number of parallel tasks leads to a strong performance loss in this context.

Enabling multithreading implies, on the one hand, that the services are able to process many parallel connections and, on the other hand, that the workflow engine is able to submit several simultaneous

queries to a service leading to the dynamic creation of several threads. Moreover, a multithreaded workflow engine should implement a dedicated data management system. Indeed, in case of a multithreaded execution, a data is able to overtake another one during the processing and this could lead to a causality problem, as we explained in [2]. To properly tackle this problem, data provenance has to be monitored during the multithreaded execution. Detailed work on data provenance can be found in [24].

Consider the simple workflow made of 3 services and represented on figure 2. Suppose that we want to execute this workflow on 3 independent input data sets D_0 , D_1 and D_2 . The multithreaded execution diagram of this workflow is represented on figure 3. On this kind of diagrams, the abscissa axis represents time. When a data set D_i appears on a row corresponding to a service P_j , it means that D_i is being processed by P_j at the current time. To facilitate legibility, we represented with the D_i notation the piece of data resulting from the processing of the initial input data set D_i all along the workflow. For example, in the diagram of figure 3, it is implicit that on the P_2 service row, D_0 actually denotes the data resulting from the processing of the input data set D_0 by P_1 . On those diagrams, we moreover made the assumption that the processing time of every data set by every service is constant, thus leading to cells of equal widths. Multithreading occurs when different data sets appear on a single square of the diagram whereas intrinsic workflow parallelism occurs when the same data set appears many times on different cells of the same column. Crosses represent idle cycles.

The Taverna workbench [15], for example, only implements a limited multithreading strategy. The user can specify a *fixed* number of threads *limited to 10*. Such a limitation is clearly too low for a data-intensive application benefiting of a data grid, and the number cannot be dynamically adjusted by the scheduler. In [2], we presented an asynchronous framework of invocation between Taverna and Web-Services, by splitting the services into a submission and a fetching service. These services are able to cope with this limitation. Nevertheless, it is clear that this problem can only properly be solved at the workflow enactor level.

P_3	X	D_0 D_1 D_2
P_2	X	D_0 D_1 D_2
P_1	D_0 D_1 D_2	X

Fig. 3. Multithreaded execution diagram of the workflow of figure 2

C. Service parallelism – pipelining

Input data sets are likely to be independent from each other. This is for example the case when a single workflow is iterated in parallel on many input data sets. Thus, parallelism can also be highlighted at a service level in the workflow.

Pipelining denotes that the processing of two different data sets by two different services are totally independent. A workflow enactor should allow pipelining of sequential tasks, in order to optimize the workflow execution.

Pipelining has been very successfully implemented in hardware processors to reduce the time spent during the completion of sequential instructions. This model can be adapted to sequential parts of workflows. Consider again the simple workflow represented on figure 2, to be executed on the 3 independent input data sets D_0 , D_1 and D_2 . Figure 5 presents a pipelined execution diagram of this workflow whereas figure 4 displays a non pipelined one. We here supposed that a given service can only process a single data set at a given time (multithreading is disabled). On those diagrams, pipelining occurs when different data sets appear on different cells of the same column.

Here again, the Taverna workflow manager does not allow the pipelined execution of a workflow. Efforts have been done to cope with this limitation by developing specific services [25]. Nevertheless, pipelining has to be enabled by the workflow enactor itself in order to be used with standard Web-Services that provide genericness and are thus particularly adapted to our assumptions.

D. Data synchronization

Nevertheless, in some cases, different data sets need to be synchronized, in order to compute an

P_3	X	X	X	D_0	D_1	D_2
P_2	X	X	X	D_0	D_1	D_2
P_1	D_0	D_1	D_2	X	X	X

Fig. 4. Non pipelined execution diagram of the workflow of figure 2

P_3	X	D_0	D_1	D_2
P_2	X	D_0	D_1	D_2
P_1	D_0	D_1	D_2	X

Fig. 5. Pipelined execution diagram of the workflow of figure 2

operation on more than one data set. In such workflow areas, a pipelined execution cannot be used and the engine must be aware of such synchronization services. An example of such a case occurs when one need to compute statistics such as the mean of all data. It is the case in workflows such as the Bronze-Standard medical image registration assessment application that we describe in section VI and in [2].

Figure 6 displays such a synchronization pattern. The service μ corresponds to a synchronization operation that needs to be executed on the whole data. We figured it with a double square in the diagram.

IV. INFLUENCE ON THE EXECUTION TIME

In order to show how pipelining and multithreading influence the execution time of a workflow, we determine in this section the workflow execution times for a given execution policy.

A. Definitions and notations

- In the workflow, a *path* denotes a set of services linking an input to an output.
- The *critical path* of the workflow denotes the longest path in terms of execution time.



P_2	X	D_0	D_1	D_2	X
P_1	D_0	D_1	D_2	X	X
μ	X	X	X	X	D_0, D_1, D_2

Fig. 6. Example of a data synchronization pattern and its execution diagram

- n_w denotes the number of services on the critical path of the workflow.
- n_D denotes the number of data sets to be executed by the workflow.
- i denotes the index of the i^{th} service of the critical path of the workflow ($i \in \llbracket 0, n_w - 1 \rrbracket$). Similarly j denotes the index of the j^{th} data set to be executed by the workflow ($j \in \llbracket 0, n_D - 1 \rrbracket$).
- $T_{i,j}$ denotes the duration in seconds of the treatment of the data set j by the service i .
- $\sigma_{i,j}$ denotes the absolute time in seconds of the end of the treatment of the data set j by the service i . The execution of the workflow is assumed to begin at $t = 0$. Thus $\sigma_{0,0} = T_{0,0} > 0$.
- Σ denotes the total execution time of the workflow:

$$\Sigma = \max_{j < n_D} (\sigma_{n_w-1,j}) \quad (1)$$

Notations are represented on figure 7.

B. Hypotheses

- The critical path is assumed not to depend on the data set. This hypothesis seems reasonable for most applications but may not hold in some cases as for example the one of workflows including algorithms containing optimization loops whose convergence time is likely to vary in an complex way w.r.t the nature of the input data set.
- Multithreading is assumed not to be limited by infrastructure constraints. We justify this hypothesis considering that our target infrastructure is a grid, whose computing power is sufficient for our application.
- In this section, workflows are assumed not to contain any synchronization pattern (see section III-D for definition). Workflows containing such patterns may be viewed as two subworkflows respectively corresponding to the parts of the initial workflow preceding and succeeding the synchronization pattern (the synchronization pattern itself being included in the succeeding part). Execution times of those two subworkflows can be determined using the following expressions. The execution time of the global workflow will then correspond to

the sum of the execution times of the subworkflows.

C. Execution times

Under those hypotheses, we can determine the expression of the total execution time of the workflow for every execution policy:

- Case S: Sequential (pipelining and multithreading disabled):

$$\Sigma_S = \sum_{i < n_W} \sum_{j < n_D} T_{i,j} \quad (2)$$

- Case M: pipelining disabled and multithreading enabled:

$$\Sigma_M = \sum_{i < n_W} \max_{j < n_D} \{T_{i,j}\} \quad (3)$$

- Case P: pipelining enabled and multithreading disabled:

$$\Sigma_P = T_{n_W-1, n_D-1} + m_{n_W-1, n_D-1} \quad (4)$$

with: $\forall i \neq 0$ and $\forall j \neq 0$,

$$m_{i,j} = \max(T_{i-1,j} + m_{i-1,j}, T_{i,j-1} + m_{i,j-1})$$

and:

$$m_{0,j} = \sum_{k < j} T_{0,k} \quad \text{and} \quad m_{i,0} = \sum_{k < i} T_{k,0}$$

- Case PM: pipelining enabled and multithreading enabled:

$$\Sigma_{PM} = \max_{j < n_D} \left\{ \sum_{i < n_W} T_{i,j} \right\} \quad (5)$$

All the above expressions of the execution times can easily be shown recursively. Here is an example of such a proof for Σ_P .

We first can write that, for a pipelined and non-multithreaded execution:

$$\begin{aligned} \forall i \neq 0 \quad \text{and} \quad \forall j \neq 0 : \\ \sigma_{i,j} = T_{i,j} + \max(\sigma_{i-1,j}, \sigma_{i,j-1}) \end{aligned} \quad (6)$$

Indeed, if multithreading is disabled, data sets are processed one by one and service i has to wait for data set $j-1$ being processed by service i before starting processing the data set j . This expression is illustrated by the two configurations displayed on figure 7.

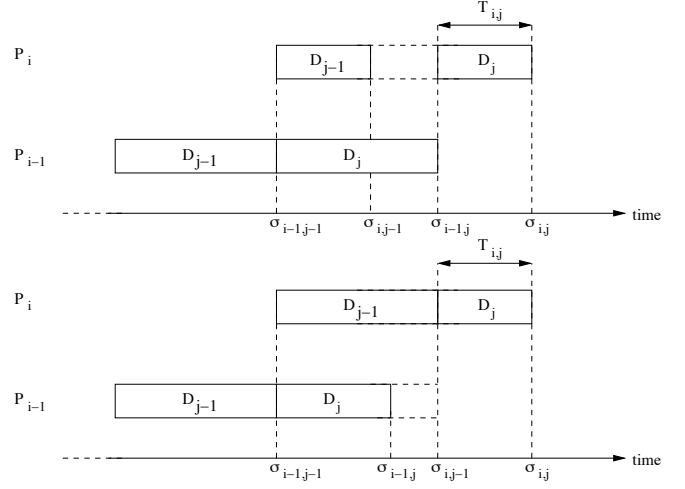


Fig. 7. Two different configurations for an execution with pipelining enabled and multithreading disabled

We moreover note that service 0 is never idle until the last data set has been processed and thus:

$$\sigma_{0,j} = \sum_{k \leq j} T_{0,k} \quad (7)$$

Furthermore, D_0 is sequentially processed by all services and thus:

$$\sigma_{i,0} = \sum_{k \leq i} T_{k,0} \quad (8)$$

We can then use the following lemma, whose proof is deferred to the end of the section:

Lemma IV.1

$$P(i, j) : \quad \sigma_{i,j} = T_{i,j} + m_{i,j}$$

with: $\forall i \neq 0$ and $\forall j \neq 0$,

$$m_{i,j} = \max(T_{i-1,j} + m_{i-1,j}, T_{i,j-1} + m_{i,j-1}),$$

and:

$$m_{0,j} = \sum_{k < j} T_{0,k} \quad \text{and} \quad m_{i,0} = \sum_{k < i} T_{k,0}$$

Moreover, we can deduce from equation 6 that for every non null integer j , $\sigma_{i,j} > \sigma_{i,j-1}$, which implies that $\Sigma_P = \sigma_{n_W-1, n_D-1}$ (according to equation 1).

Thus, according to lemma IV.1

$$\begin{aligned}\Sigma_P &= T_{n_W-1, n_D-1} + m_{n_W-1, n_D-1} \\ &\text{with: } \forall i \neq 0 \text{ and } \forall j \neq 0, \\ m_{i,j} &= \max(T_{i-1,j} + m_{i-1,j}, T_{i,j-1} + m_{i,j-1}), \\ &\text{and:} \\ m_{0,j} &= \sum_{k < j} T_{0,k} \quad \text{and:} \quad m_{i,0} = \sum_{k < i} T_{k,0}\end{aligned}$$

■

Proof of lemma IV.1: The lemma can be shown **via a double recurrence**, first on i and then on j . Recursively w.r.t i :

- **i=0**: According to equation 7:

$$\begin{aligned}\forall j < n_D, \quad \sigma_{0,j} &= \sum_{k \leq j} T_{0,k} \\ &= T_{0,j} + m_{0,j} \\ &\text{with} \\ m_{0,j} &= \sum_{k < j} T_{0,k}\end{aligned}$$

$\forall j < n_D$, $P(0,j)$ is thus true.

- Suppose H_i : $\forall j < n_D$ $P(i,j)$ true. We are going to show recursively w.r.t j that H_{i+1} is true:

- **j=0**: According to equation 8:

$$\begin{aligned}\sigma_{i+1,0} &= \sum_{k \leq i+1} T_{k,0} \\ &= T_{i+1,0} + m_{i+1,0} \\ &\text{with} \\ m_{i+1,0} &= \sum_{k < i+1} T_{k,0}\end{aligned}$$

H_{i+1} is thus true for $j = 0$.

- Suppose K_j : H_{i+1} is true for j . We are going to show that K_{j+1} is true.

According to equation 6:

$$\sigma_{i+1,j+1} = T_{i+1,j+1} + \max(\sigma_{i,j+1}, \sigma_{i+1,j})$$

Thus, according to K_j :

$$\begin{aligned}\sigma_{i+1,j+1} &= T_{i+1,j+1} \\ &\quad + \max(\sigma_{i,j+1}, T_{i+1,j} + m_{i+1,j})\end{aligned}$$

And, according to H_i :

$$\begin{aligned}\sigma_{i+1,j+1} &= T_{i+1,j+1} + \\ &\quad \max(T_{i,j+1} + m_{i,j+1}, \\ &\quad T_{i+1,j} + m_{i+1,j})\end{aligned}$$

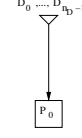


Fig. 8. Massively data-parallel workflow pattern

$$= T_{i+1,j+1} + m_{i+1,j+1}$$

with:

$$\begin{aligned}m_{i+1,j+1} &= \max(T_{i,j+1} + m_{i,j+1}, \\ &\quad T_{i+1,j} + m_{i+1,j})\end{aligned}$$

K_{j+1} is thus true.

H_{i+1} is thus true.

The lemma is thus true. ■

D. Speed-ups

In this section, we study the asymptotic speed-ups introduced by pipelining and multithreading.

1) *Massively data-parallel workflows*: Let us consider a massively data-parallel workflow as the one represented in figure 8. In such workflows, $n_W = 1$ and the execution times resume to:

$$\Sigma_M = \Sigma_{PM} = \max_{j < n_D} (T_{0,j}) \ll \Sigma_S = \Sigma_P = \sum_{j < n_D} T_{0,j}$$

In this case, multithreading leads to a significant speed-up. Pipelining is useless but do not lead to any overhead.

2) *Data non intensive workflows*: In such workflows, $n_D = 1$ and the execution times resume to:

$$\Sigma_M = \Sigma_{PM} = \Sigma_S = \Sigma_P = \sum_{i < n_W} T_{i,0}$$

In this case, neither multithreading nor pipelining lead to any speed-up. Nevertheless, neither of them do introduce any overhead.

3) *Data intensive complex workflows*: In this case, we will suppose that:

$$n_D \rightarrow \infty \quad \text{and:} \quad n_W > 1$$

In order to analyze the speed-ups introduced by pipelining and multithreading in this case, we make

the simplifying assumption of constant execution times:

$$T_{i,j} = T \quad (9)$$

In this case, the workflow execution times resume to:

$$\begin{aligned} \Sigma_M = \Sigma_{PM} &= n_W \times T \\ \Sigma_S &= n_D \times n_W \times T \\ \Sigma_P &= (n_D + n_W - 1) \times T \end{aligned}$$

Those expressions can be checked on the execution diagrams of section III.

Pipelining do not lead to any speed-up in addition to multithreading. However, we will see in section VI-D that T is hardly constant in production systems and that in this case the conclusion does not hold. Indeed, figures 9 and 10 illustrate on a simple example that pipelining do provide a speed-up even if multithreading is enabled, if the assumption of constant execution times is not done.

If multithreading is disabled, the induced speed-up is:

$$S = \frac{n_D \times n_W}{n_D + n_W - 1}$$

In case of data intensive workflows, this speed-up is significant. Indeed:

$$\lim_{n_D \rightarrow +\infty} S = n_W$$

Moreover, this speed-up is growing with the number of input data sets. Indeed:

$$\frac{dS}{dn_D} = \frac{n_W \cdot (n_W - 1)}{(n_D + n_W - 1)^2} \quad (10)$$

This derivative is always positive but decreases to zero when n_D tends towards infinity. This speed-up is thus smoothly growing with the number of input data sets.

We can conclude from this section that pipelining leads to a significant speed-up for the execution of a data-intensive complex workflow. This kind of workflow is the one targeted by our application. That is why we focus on the implementation of a workflow enactor that enables pipelining in the rest of the paper.

P_3	X	X	D_2 D_1 D_0	X	X
P_2	X	X	D_0 D_2 D_1	D_1	D_1
P_1	D_2 D_1 D_0	D_0	X	X	X

Fig. 9. Multithreaded non pipelined execution diagram of the workflow of figure 2 with the assumption of variable execution times.

P_3	X	D_1 D_2	D_0	X
P_2	X	D_2 D_1	D_0 D_1	D_1
P_1	D_2 D_1 D_0	D_0	X	X

Fig. 10. Multithreaded pipelined execution diagram of the workflow of figure 2 with the assumption of variable execution times. Comparing this diagram to the one of figure 9, one can see that pipelining do provide a speed-up even if multithreading is enabled if the execution times are not constant.

V. IMPLEMENTATION OF A PROTOTYPE

We implemented a prototype of a workflow enactor taking into account the 3 kinds of parallelism we described in section III: intrinsic workflow parallelism, multithreading and pipelining. Our home-made OpTimisEd scUfl enactor (MOTEUR) prototype was implemented using Java, in order to make it platform independent. It is available under CeCILL Public License (a GPL-compatible open source license) at <http://www.i3s.unice.fr/~glatard>.

A. Workflow description language

This prototype is able to enact a workflow of standard Web-Services described with the Simple Concept Unified Flow Language (ScUfl) used by the Taverna workbench [15]. This language is currently becoming a standard in the e-Science community.

Apart from describing the data links between the services, this language allows to define so-called coordination constraints. A coordination constraint is a control link which enforce an order of execution between to services even if there is no data dependency between them. We used those coordination

constraints to identify services that require data synchronization.

The Scuf language also specifies the number of threads of a service. In our case, this number is dynamically determined during the execution, with respect to the available input data of the service, so that we only consider that a service is multithreaded or not.

B. Input data description

We developed an XML-based language to be able to describe input data sets. This language aims at providing a file format to save and store the input data set in order to be able to re-execute workflows on the same data set. It simply describes each item of the different inputs of the workflow.

C. Enactor model

The UML class diagram of the prototype we implemented is represented on figure 14.

a) *Data management*: Services have input and output ports. Each port has children ports, so that a service can convey data from its output ports directly to the corresponding children ports, without going via the central workflow entity.

Data also has parents and children data: when a new data is produced by a service, it is appended to each piece of data that was used to produce it. Thus, this provides a basic mechanism to retrieve data provenance of a result at the end of the workflow execution by going back in the data tree. Handling data provenance is particularly crucial in multithreaded workflows, as we explained in section III-B.

The Scuf language specifies so-called *iteration strategies* to handle input data of the services. An iteration strategy is a composition of two kinds of binary operators, *cross product* and *dot product*. Let us consider two inputs A and B of a service P, each of them being instantiated by a fixed number of data sets: A_0, A_1, \dots, A_n for input A and B_0, B_1, \dots, B_m for input B. If the iteration strategy of this service P is a *cross product*, then P will process each A_i with every B_j ($i < n$ and $j < m$), thus leading to $n \times m$ computations. Conversely, if the iteration strategy of P is a *dot product*, then P will process each A_i with the corresponding B_i , thus leading to n computations (one must then have $n = m$ and $i < n$) (cf. figure 11 for details).

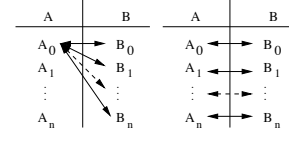


Fig. 11. Action of the *cross product* (left) and *dot product* (right) operators on the input data

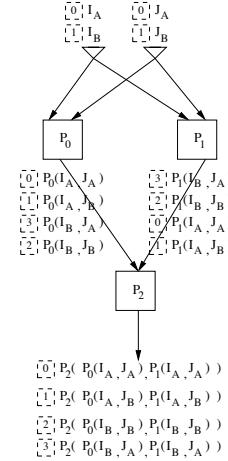


Fig. 12. Example illustrating the need for a unique identification of data sets in a multithreaded workflow: services P_0 and P_1 compute *cross products* on their input data whereas service P_2 computes a *dot product*. Without any appropriate numbering (represented in dotted lines cells here), P_2 may not process the right dot product because P_0 and P_1 are multithreaded and produce their result in a different order. $P_i(I, J)$ denotes the result of the processing of data sets I and J by service P_i

Handling iteration strategies in a multithreaded pipelined workflow is not straightforward because produced data sets have to be uniquely identified. Indeed they are likely to be computed in a different order in every service, which could lead to wrong dot product computations, as figure 12 illustrates. Moreover, due to pipelining, several data sets are processed concurrently and one cannot number all the produced data once computations completed. Thus, we use the following bijective function f to number the data produced by *cross products*:

$$f : \mathbb{N} \times \mathbb{N} \rightarrow \mathbb{N}$$

$$(i, j) \mapsto k^2 + k + i - j$$

where $k = \max(i, j)$

This function is injective, which guarantee the uniqueness of the numbering. Here is the proof of

the injectivity of f . We first can note that for every integer n , there is a *unique* integer k_n such as:

$$k_n^2 \leq n < (k_n + 1)^2 \quad (11)$$

Moreover it is obvious that:

$$\forall (x, y) \in \mathbb{N}^2, \quad k^2 \leq f(x, y) < (k + 1)^2 \quad (12)$$

with $k = \max(x, y)$

Suppose that we have (x_0, y_0) and (x_1, y_1) two pairs of integers such as $f(x_0, y_0) = f(x_1, y_1)$. We are going to show that $(x_0, y_0) = (x_1, y_1)$. Let $k_0 = \max(x_0, y_0)$ and $k_1 = \max(x_1, y_1)$. According to equation 12, we have:

$$k_0 \leq f(x_0, y_0) < (k_0 + 1)^2 \quad \text{and} \\ k_1 \leq f(x_1, y_1) < (k_1 + 1)^2$$

Moreover, according to equation 11, there is a unique integer k such as:

$$k^2 \leq f(x_0, y_0) = f(x_1, y_1) < (k + 1)^2$$

Thus, given the uniqueness of k , we have $k_0 = k_1 = k$. We then have:

$$(k = x_0 \quad \text{OR} \quad k = y_0) \quad \text{AND} \quad (k = x_1 \quad \text{OR} \quad k = y_1)$$

This leads to 4 distinct cases:

- 1) $k = x_0$ AND $k = x_1$:
Thus: $k^2 + k + k - y_0 = k^2 + k + k - y_1$ and $y_0 = y_1$.
- 2) $k = y_0$ AND $k = y_1$:
As well as case 0, $x_0 = x_1$.
- 3) $k = x_0$ AND $k = y_1$:
Thus: $x_1 + y_0 = 2k$
Finally: $x_1 = y_0 = k$ because $y_0 \leq k$ and $x_1 \leq k$.
- 4) $k = x_1$ AND $k = y_0$:
As well as case 3, $x_0 + y_1 = 2k$ and $x_0 = y_1 = k$ because $x_0 \leq k$ and $y_1 \leq k$.

We thus have $(x_0, y_0) = (x_1, y_1)$ for each of those cases. ■

Actually, this function corresponds to the numbering of \mathbb{N}^2 displayed on figure 13. This function is also surjective (and thus bijective) as it can be intuited from figure 13.

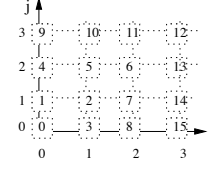


Fig. 13. Numbering used to label the data in the workflow. The values of f are displayed in the cells.

b) Services enactment: A workflow contains a list of services and is responsible for their enactment (`process()` method on the UML diagram of figure 14), so that the execution control is centralized in a single entity. The workflow queries services to check whether they are ready to be enacted (`isReady()` method on figure 14). Services answer depending on the data available in their input ports and on the status of the elements of the `toWait` attribute.

This attribute aims at enabling data synchronization, as explained in section III-D. In the implemented enactment strategy, a service will wait for every service S in the `toWait` array and recursively for every ancestor of S to be inactive before starting. This implementation of data synchronization is limited but suitable for our application as we will see in section VI. Other kinds of synchronization could of course be defined, to impose services to wait for a particular piece of data produced by its parents, taking into consideration the data-tree described in the previous paragraph. However, this would require to be able to express such synchronization strategies with the Scuf language, which is not the case yet since only a single kind of so-called coordination constraint is available.

Sources and sinks are particular "Nop" services which do not process anything and just convey data from their single input port to their single output port.

VI. EXPERIMENTS

A. Application

We made experiments considering a medical imaging rigid registration application. Medical image registration consists in searching a transformation (that is to say 6 parameters in the rigid case – 3 rotation angles and 3 translation parameters)

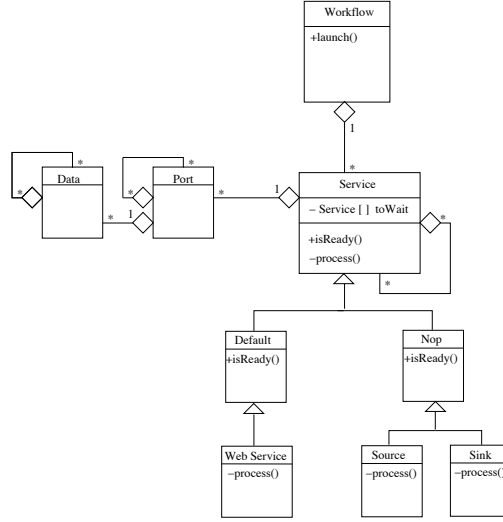


Fig. 14. UML diagram of the prototype we implemented

between two images, so that the first one (the floating image) can superimpose on the second one (the reference image) in a common 3D frame. Medical image registration algorithms are a key component of medical imaging workflows.

The application we are working on aims at assessing registration results with a statistical approach called the Bronze-Standard [26]. The goal is basically to compute the registration of a maximum of image pairs with a maximum number of registration algorithms so that we obtain a largely overestimated system to relate the geometry of all the images. As a consequence, the mean registration should be more precise and is called a bronze-standard. It implies that we are first able to process registrations of many pairs of images, which is a data-intensive problem.

The workflow of our application is represented on figure 15. The two inputs `referenceImage` and `floatingImage` correspond to the image sets on which the evaluation is to be processed. The first registration algorithm is `crestMatch`. Its result is used to initialize the other registration algorithms which are `Baladin`, `Yasmina` and `PFMatchICP/PFRegister`. `crestLines` is a pre-processing step. Then, the `formatConversion` and `writeResults` services are executed locally and aim at recording the results in a suitable format. Finally, the `MultiTransfoTest` service is responsible for the evaluation of the accuracy of

the registration algorithms, leading to the outputs values of the workflow. This evaluation considers means computed on all the results of the registration services except one that we specify and evaluates the accuracy of the specified method. Thus, the `MultiTransfoTest` service has to be synchronized: it must be enacted once every of its ancestor is inactive. This is why we figured it with a double square on figure 15.

As detailed in section VI-C, we made experiments on two different infrastructures: a local one, made of 4 PCs and the EGEE grid one. Corresponding workflows are both identical, except that a `getFromEGEE` service has been added on the EGEE workflow, in order to download results from the grid *at the end* of the registration procedures. Other steps in the workflow do not need such a service because data transfers within the grid are handled by the grid middleware itself.

B. Data

Input image pairs are taken from a database of injected T1 brain MRIs from the cancer treatment center "Centre Antoine Lacassagne" in Nice, France (courtesy of Dr Pierre-Yves Bondiau). All images are 256×256×60 and coded on 16 bits, thus leading to a 7.8 MB size per image (approximately 2.3 MB when compressed).

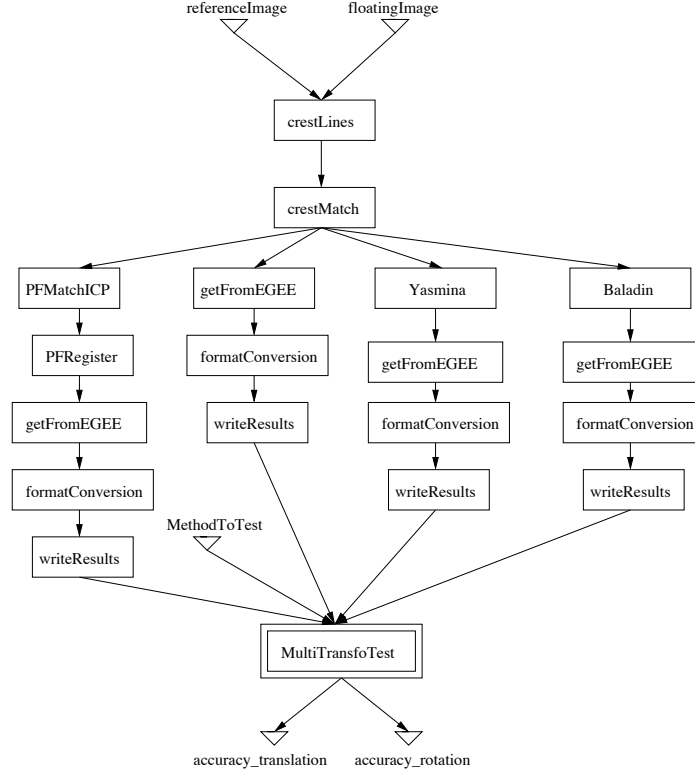


Fig. 15. Workfbw of the application

C. Experimental terms

We made experiments in order to evaluate the relevance of our prototype on two different infrastructures. These infrastructures correspond to different parallelism conditions. On each infrastructure, we measured the workflow execution time for various numbers of input data sets.

We first deployed our application on an *local infrastructure*, where a single monoprocessor machine is dedicated to each registration algorithm. Intrinsic workflow parallelism and pipelining do make sense on this infrastructure, whereas multithreading does not. Indeed, in case of multithreading, multiple instances of a service would be executed on a single physical processor, which would not lead to any execution speed-up.

We also deployed the application on the *grid infrastructure* provided by the EGEE European project. The platform offered is a pool of thousands computing (standard PCs) and storage resources

accessible through the LCG2 middleware⁵. The resources are assembled in computing centers, each of them running its internal batch scheduler. Jobs are submitted from a user interface to a central Resource Broker which distributes them to the available resources. Not only intrinsic workflow parallelism and pipelining but also multithreading make sense on such a grid infrastructure. Indeed, every instance of a service will be submitted to the grid and thus executed on a different processor.

In both cases, we compared execution times with and without pipelining. We used our MOTEUR for the pipelined case and for the non pipelined case, we used the Freefluo⁶ enactor, which is the one included into the Taverna workbench. Because of a limitation of this workbench, the number of threads was limited to 10 with this enactor.

For each of the above infrastructures, we executed our workflow on 3 inputs data sets, corresponding to

⁵<http://lcg-web.cern.ch>

⁶<http://freefluo.sourceforge.net>

the registration of 12, 66 and 126 image pairs from the database described in section VI-B. These inputs data sets correspond respectively to images from 1, 7 and 25 patients on which acquisitions have been done at several time points to monitor the growth of brain tumors. Each of the input image pair was registered with the 4 algorithms, thus respectively leading to 48, 264 and 504 registrations.

D. Results

1) *Evaluation of our MOTEUR on the local infrastructure*: Table I displays the comparison between the execution times obtained with Taverna and our MOTEUR on the local infrastructure w.r.t the number of input data sets. S_p denotes the speed-up introduced by the pipeline strategy implemented in our prototype. On this infrastructure, our prototype introduces an average speed-up of 1.74 w.r.t the execution with Taverna. This speed-up is smoothly growing with the number of input data sets, as predicted by equation 10.

Moreover, one can notice on figure 16 that execution times are a linear function of the size of the input data set on this local infrastructure. This function is a straight line because of the nature of the workflow which iterates the same computations on each data set. It tends towards zero when n_D tends towards zero thanks to the low latency of the local infrastructure.

2) *Evaluation of our MOTEUR on the EGEE infrastructure*: Table II displays the comparison between the execution times obtained with Taverna and our MOTEUR on the EGEE infrastructure w.r.t the number of input data sets. On this infrastructure, our MOTEUR introduces an average speed-up of 2.03 w.r.t the execution with Taverna. This speed-up is growing with the number of input data sets.

Section IV-D predicted a speed-up of 1 for our prototype on such a multithreaded environment. This is not the case here. It can be explained by the fact that the hypothesis of constant execution times (cf. equation 9) may not be verified here because of the highly variable nature of the grid environment. Indeed, on a production grid infrastructure such as the EGEE one, the multi-users system is permanently under unpredictable load. Thus, a few jobs are likely to remain blocked for a while on a particular area of the system (such as a waiting

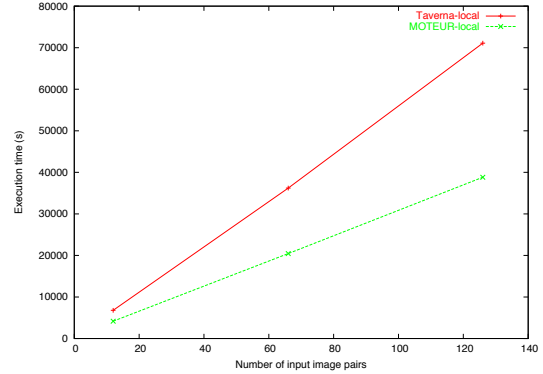


Fig. 16. Execution times of MOTEUR vs Taverna on the **local infrastructure**

queue), whereas other ones are faster to execute. And even if their proportion remains reasonable, “outlier” jobs can be very late with respect to the faster ones, thus leading to a high variability of execution times among jobs and consequently to a strong delay of the workflow if the execution is not pipelined. Future work [27] will try to model this variability in order to cope with it.

We can also clearly notice on figure 17 that the extrapolation of those curves would not give a zero value for $n_D = 0$. This can be explained by the high latency introduced by the grid. The consequences of this latency can be viewed on figures 18 and 19. We can clearly see on those figures that with Taverna as well as with our MOTEUR, our application is slowed down by the execution on the EGEE grid for low numbers of input data.

More measures remains to be done in order to present statistics concerning execution times on this infrastructure instead of just one experimental result. This is part of our future work.

We can thus conclude from those results that our MOTEUR is particularly suitable for executions of data-intensive applications in grid environments.

VII. CONCLUSION AND FUTURE WORK

We designed a complete prototype of an optimized workflow enactor that provides significant speed-up for the execution of data-intensive workflows on a grid infrastructure. The implemented prototype is able to deal with existing standard workflows and services description languages. It benefits from computation parallelization at different levels (inherent to the workflow, data parallelism

Input Data		Execution times (s)		S_P
Number of input image pairs	Number of registration	Pipelining disabled (Taverna)	Pipelining enabled (MOTEUR)	
12	48	6789s	4160s	1.63
66	264	36217s	20457s	1.77
126	504	71095s	38816s	1.83

TABLE I
EXECUTION TIMES WITHOUT MULTITHREADING (LOCAL INFRASTRUCTURE)

Input Data		Execution times (s)		S_P
Image pairs number	Registrations number	Pipelining disabled (Taverna)	Pipelining enabled (MOTEUR)	
12	48	9959s	5906s	1.69
66	264	20073s	9922s	2.02
126	504	33662s	14220s	2.37

TABLE II
EXECUTION TIMES WITH MULTITHREADING ON (EGEE INFRASTRUCTURE)

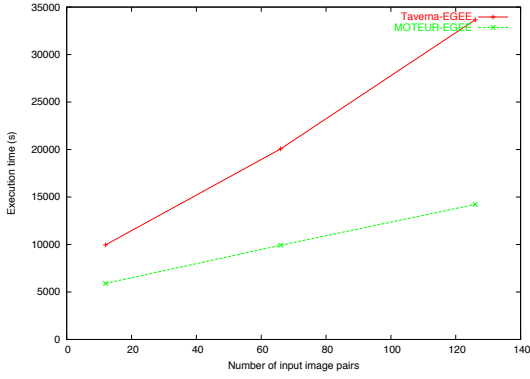


Fig. 17. Execution times of MOTEUR vs Taverna on the **EGEE infrastructure**

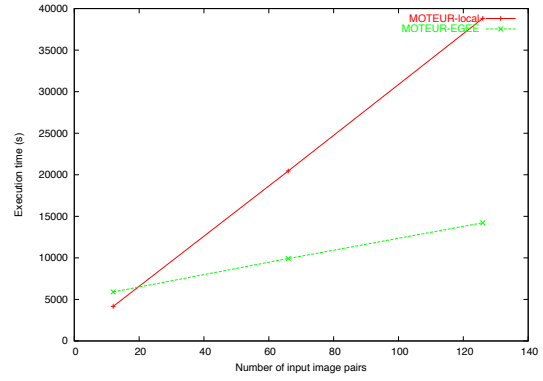


Fig. 19. Execution times of **MOTEUR** on EGEE vs on the local infrastructure. One can see that for less than 20 input image pairs, the latency of the EGEE infrastructure slows down the execution.

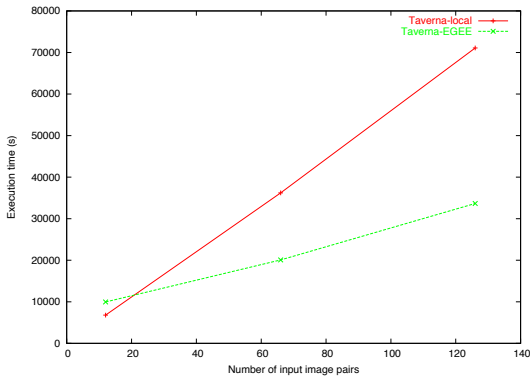


Fig. 18. Execution times of **Taverna** on EGEE vs on the local infrastructure. One can see that for less than 20 input image pairs, the latency of the EGEE infrastructure slows down the execution.

and processing parallelism) in order to exploit the resources available on grid infrastructures better than most existing implementations. The modeling of the overall execution times demonstrates that in different scenarios, the workflow manager does never lead to performance drops and that it is particularly efficient for dealing with data-intensive applications. This is confirmed by an experiment on a medical image registration application.

We have plans for further optimizing the workflow engine. To take into account the limited amount of resources really available we plan to study dynamic multithreading by adapting the number of

threads of a service to the current status of (i) the target grid infrastructure and (ii) the workflow execution. This would require to be able to monitor the status of the grid and to predict the services execution time on the infrastructure. By doing that, we plan to propose strategies to avoid pipeline draining during the workflow execution.

VIII. ACKNOWLEDGMENT

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